

# Simulation of the conversion and transport of biogenic VOC within and above forest canopies with the one-dimensional canopy-chemistry model CACHE

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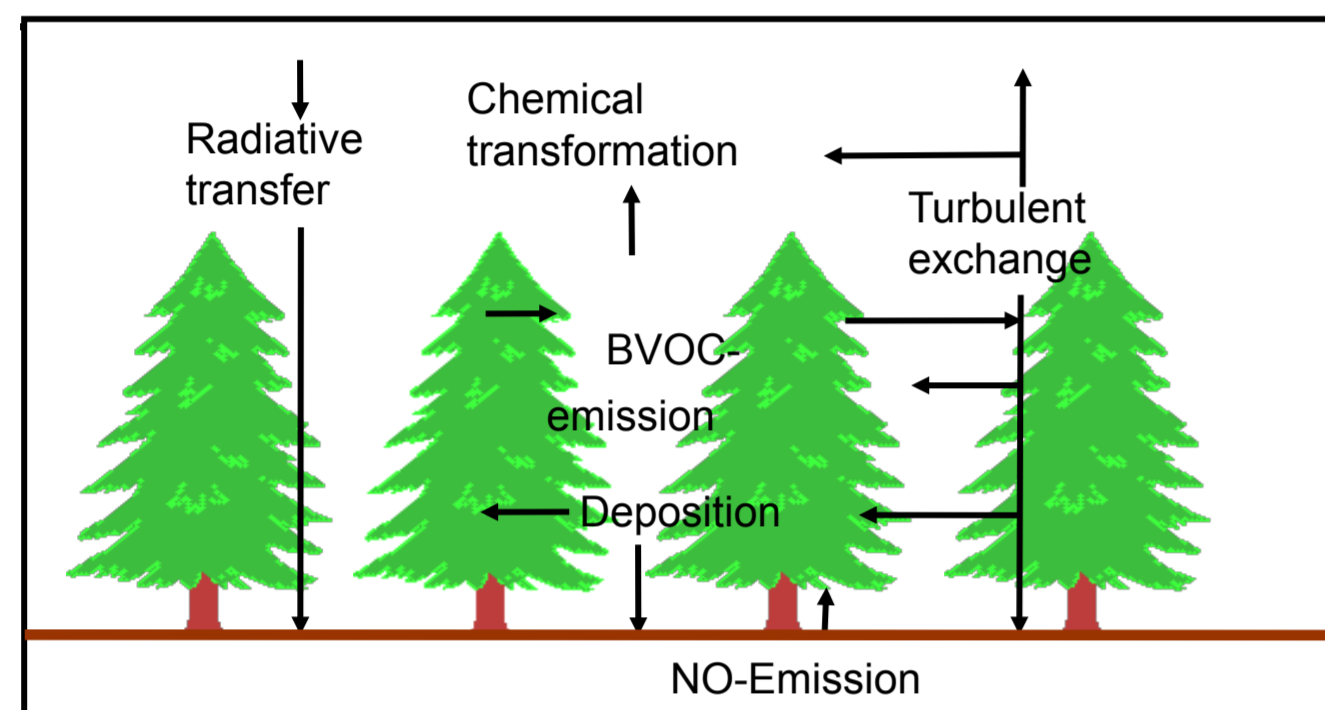
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## Introduction

Chemical reactions within and directly above tree canopies may affect the fluxes of isoprene and monoterpenes into the atmosphere and subsequent photooxidant formation. Therefore, emission rates for biogenic VOCs which are measured or computed on a leaf or branch basis may not reflect the true emission from the canopy into the boundary layer.



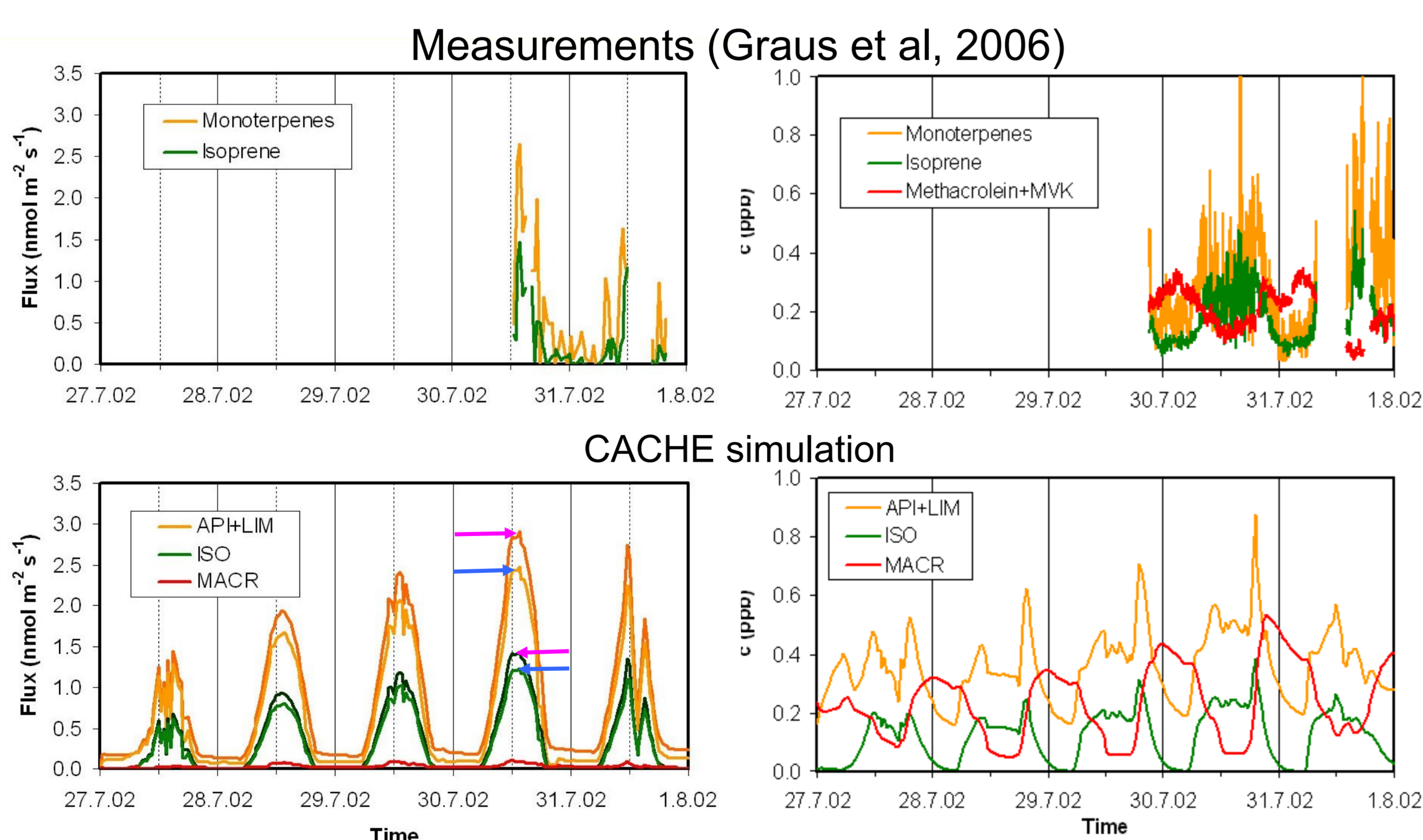
The one-dimensional multilayer canopy-chemistry model CACHE (Canopy Atmospheric CHEMistry Emission model, Forkel et al. 2006) permits the investigation of these processes within and above forest canopies:

## Model description

Starting from specified initial conditions CACHE predicts profiles of temperature, humidity, and chemical species. CACHE includes the energy balance at the leaf surfaces, turbulent transport of heat, water vapour, and gas phase chemical compounds within and above the canopy, heat and moisture transport in the soil, emission of biogenic VOC, chemical transformation, and deposition. In its standard configuration, chemical transformations are computed with the RACM gas phase chemistry mechanism of Stockwell et al. (1997).

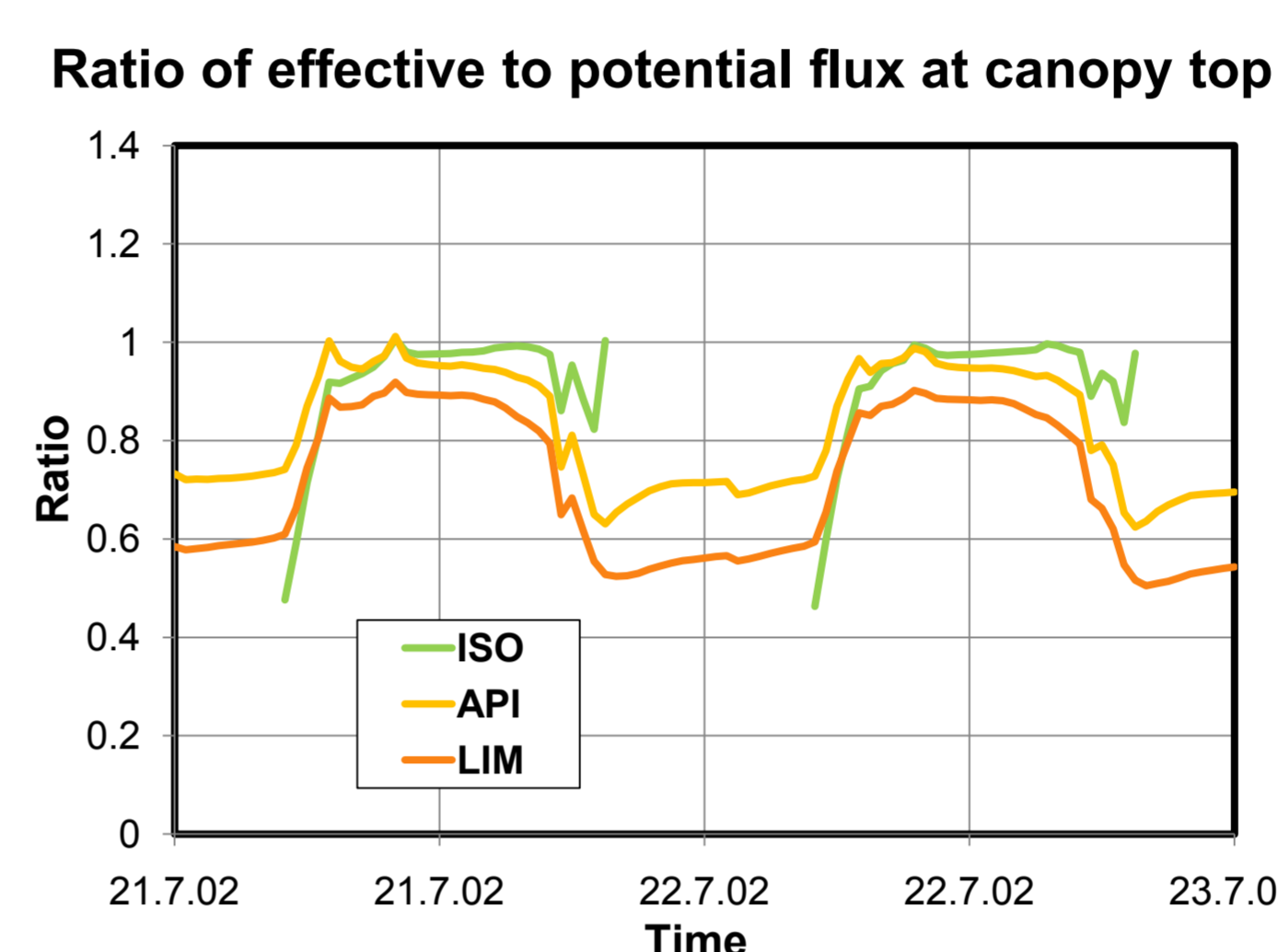
CACHE has been applied and validated for several boreal and Mediterranean forest sites. Recently CACHE has been implemented into the biosphere modeling framework MOBILE (Grote et al., 2009).

## Model validation



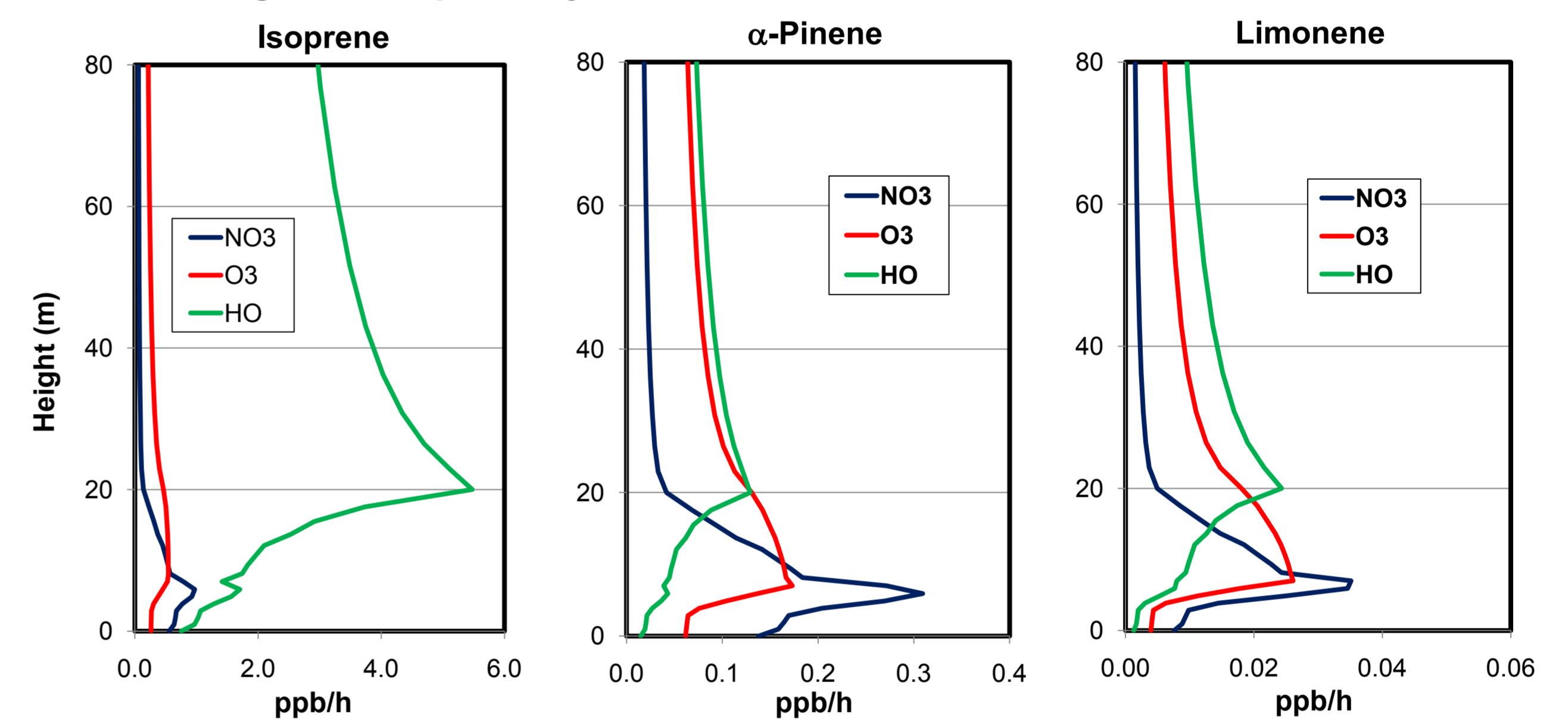
Course of observed BVOC concentrations and fluxes above a spruce forest is reproduced by the simulations. The blue arrows indicate the effective fluxes above the canopy, the red ones the potential fluxes, i.e. the fluxes calculated on branch basis.

## Results

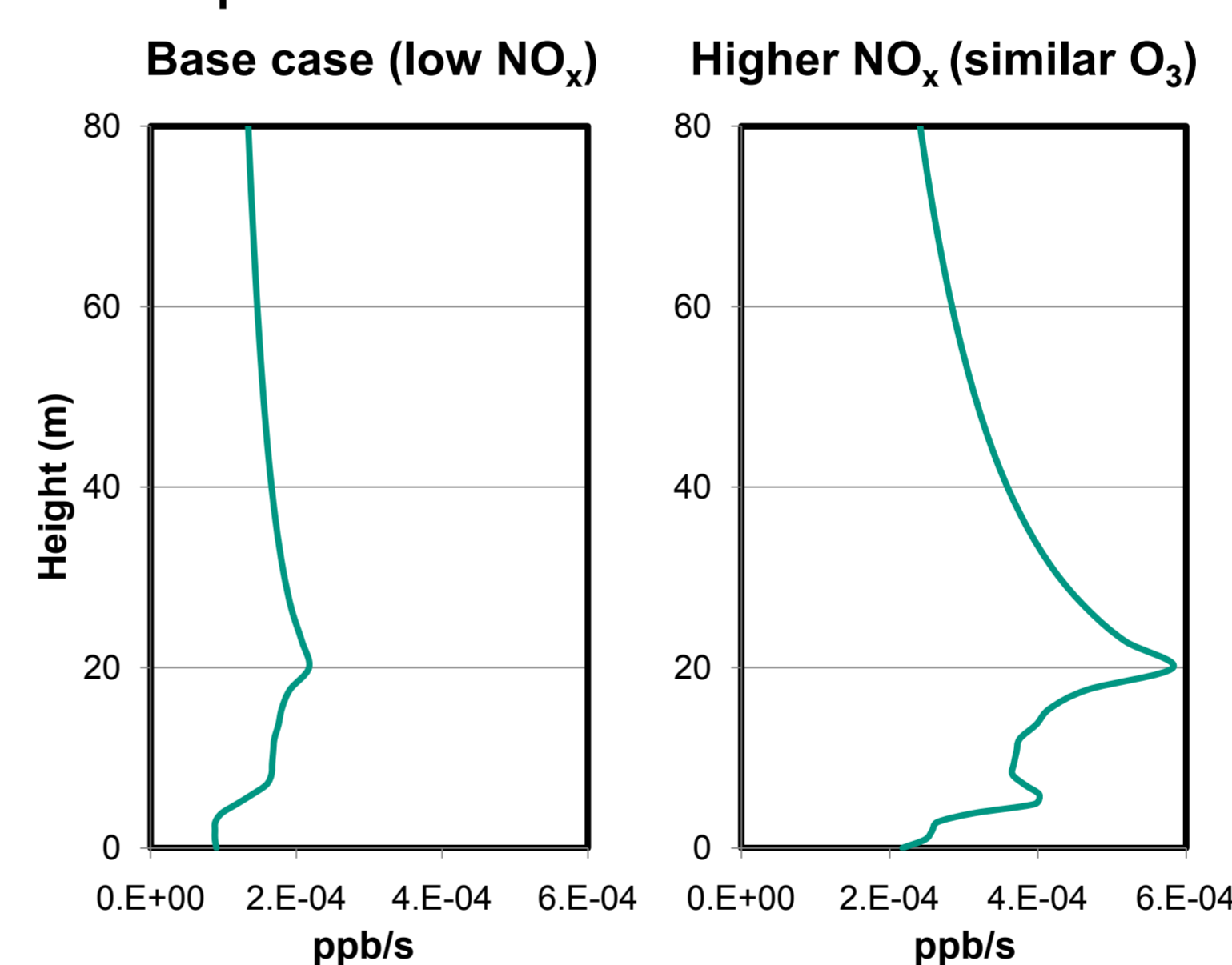


Simulated effect of in-canopy chemistry on fluxes: Depending on reactivity and residence time, BVOC fluxes into the atmosphere are 5-30 % lower than the potential fluxes (current example: American oak forest, Fuentes et al., 2007).

### BVOC degradation pathways in and above an American oak forest at noontime



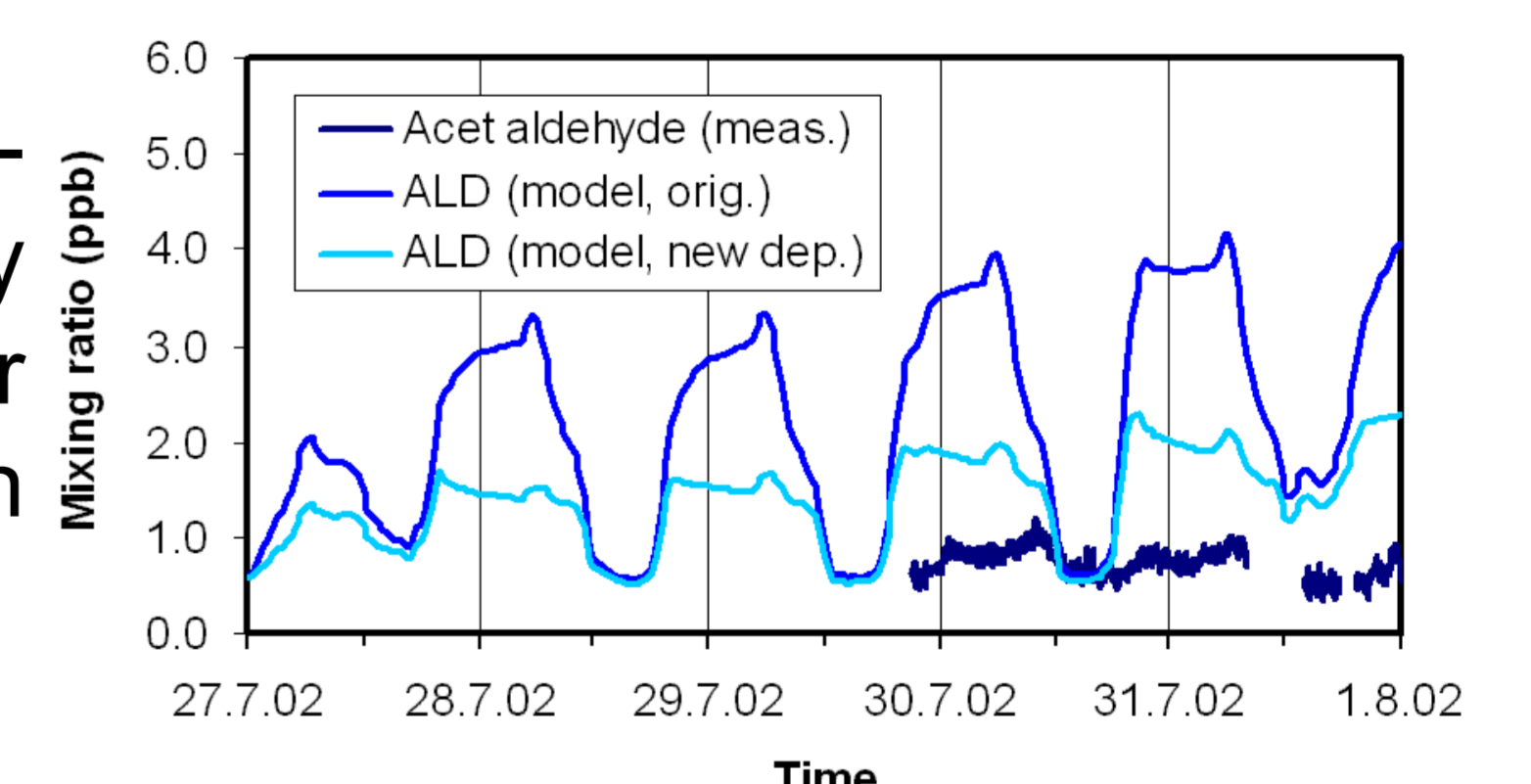
Radical reactions within and above the canopy: terpene degradation by  $\text{NO}_3$  radicals can occur also during daytime in the trunk space.



Effect of  $\text{NO}_x$  on methacrolein formation (current example: noon time, American oak forest).

For the investigation of particulate products an aerosol module is going to be implemented.

Deposition of oxygenated compounds was underestimated by the standard approach: better agreement if consumption on leaf surfaces is assumed.



## Summary

Case studies with CACHE can help to analyze the diurnal course of BVOC and product concentrations with respect to chemical reactions, mixing, and deposition and to identify open questions more clearly.

## References

- Forkel et al., 2006, *Atmospheric Environment*, 40, S28-S42.
- Fuentes et al., 2007, *J. Atmos Chem.*, 56, 165-185.
- Graus et al., 2006, *Atmospheric Environment*, 40, S28-S42.
- Grote et al., 2009, *Physics and Chemistry of the Earth*, 34, 251-260.
- Stockwell et al., 1997, *J. Geophys. Research*, 102, 25847-25879.